

2D and 3D cubic monocrystalline and polycrystalline materials: their stability and mechanical properties

C. Jasiukiewicz, T. Paszkiewicz, S. Wolski

Faculty of Mathematics and Applied Physics, Rzeszów University of Technology, ul. W. Pola 1, PL-35-959 Rzeszów, Poland

E-mail: czjas@prz.edu.pl, tapasz@prz.edu.pl, wolan@prz.edu.pl

Abstract. We consider 2- and 3-dimensional cubic monocrystalline and polycrystalline materials. Expressions for Young's and shear moduli and Poisson's ratio are expressed in terms of eigenvalues of the stiffness tensor. Such a form is well suited for studying properties of these mechanical characteristics on sides of the stability triangles. For crystalline high-symmetry directions lines of vanishing Poisson's ratio are found. These lines demarcate regions of the stability triangle into areas of various auxeticity properties. The simplest model of polycrystalline 2D and 3D cubic materials is considered. In polycrystalline phases the region of complete auxetics is larger than for monocrystalline materials.

1. Introduction

In our recent papers we considered mechanical characteristics of 3D crystalline structures of high and middle symmetry [1] and of all 2D symmetry systems [2]. In particular we derived explicit expressions for Young's E and shear G moduli as well as for Poisson's ratio ν depending on directional cosines of angles between directions \mathbf{n} of the load and the direction \mathbf{m} of the lateral strain, respectively, and directions of the crystalline symmetry axes.

Our particular attention was paid to 3D and 2D cubic structures [3], [4]. All initially unstrained quadratic and cubic materials are characterized by three parameters s_1 , s_2 and s_3 belonging to a half-infinite ($s_1 > 0$) prisms with (stability) triangles (ST) in the base lying in the (s_2, s_3) -plane.

Among mechanical characteristics, Poisson's ratio ν is particularly interesting because the phenomenon of a negative ν , i.e. solids expanding transversely to applied tensile stress, is counterintuitive. Elastic materials with negative ν are termed auxetics. Materials with negative ν for all pairs of vectors \mathbf{n} , \mathbf{m} are *complete* auxetics. Materials are auxetics if there exist pairs of \mathbf{n} , \mathbf{m} for which $\nu < 0$. Materials are non-auxetics if $\nu > 0$ for all pairs of vectors \mathbf{n} , \mathbf{m} . In papers [3], [4] we established regions of ST in which crystalline cubic and quadratic materials are completely auxetic, auxetic and non-auxetic. One may expect that complete auxetics are particularly promising from the standpoint of technology.

Many technically important materials are polycrystalline. In view of potential applications of crystalline auxetic materials, the question how polycrystallinity influences the auxetic properties deserves some attention.

The elastic properties of polycrystalline materials depend on the single-crystal stiffnesses (elastic constants) of the crystallites which build up the polycrystal and on the manner in which

crystallites are connected. In most cases exact orientations, shapes and connections are not known. These gaps in knowledge can be overcome with the help of orientation and grain shape distribution functions. Generally, one has to resort to more or less realistic assumptions (cf. [5]). We assume that the grains have the same shape and volume and that their orientations are completely random.

2. The stability conditions for initially unstressed crystalline quadratic and cubic media

Mechanical properties of crystalline materials depend on components of the stiffness tensor \mathbf{C} or on the components of the compliance tensor \mathbf{S} . These tensors are mutually inverse, i.e.

$$\mathbf{C}\mathbf{S} = \mathbf{S}\mathbf{C} = \mathbf{I}_4, \quad (1)$$

where $(\mathbf{I}_{ij,kl}^{(4)}) = (\delta_{ik}\delta_{jl} + \delta_{ij}\delta_{kl})/2$. The product of two fourth rank tensors A and B has components $(\mathbf{A}\mathbf{B})_{ijkl} = \sum_{r,s=1}^3 A_{ij,rs} B_{rs,kl}$.

In this paper we consider only 2D and 3D cubic crystalline or polycrystalline materials. For mechanically stable initially unstrained materials both \mathbf{C} and \mathbf{S} tensors are positive, therefore their eigenvalues c_I, s_I ($I = J, L, M$) are positive too ([1], [2], [6])

$$c_I > 0, s_I > 0 \quad (I = J, M, L). \quad (2)$$

Because of Eq. (1) $s_I = c_I^{-1}$ vanishing eigenvalues c_I ($I = J, L, M$) signal instabilities related to phase transitions [7].

In the case of quadratic materials [2]

$$c_J = C_{11} + C_{12}, \quad c_L = C_{11} - C_{12}, \quad c_M = 2C_{66}. \quad (3)$$

In the case of cubic materials [1], [6]

$$c_J = C_{11} + 2C_{12}, \quad c_L = C_{11} - C_{12}, \quad c_M = 2C_{66}. \quad (4)$$

In Eqs. (3) and (4) we used the familiar Voigt's notation [8]: $C_{11} = C_{11,11}$, $C_{12} = C_{11,22}$ and $C_{66} = C_{12,12}$.

For cubic materials a more reasonable choice of independent parameters was proposed by Every [9] and for quadratic materials in our paper [4]

$$\begin{aligned} s_1 &= C_{11} + (d-1)C_{66}, \quad s_2 = \frac{C_{11} - C_{66}}{s_1}, \\ s_3 &= \frac{C_{11} - C_{12} - 2C_{66}}{s_1}, \end{aligned} \quad (5)$$

where $d = 2$ for 2D, $d = 3$ for 3D materials.

We rewrite expressions (3) and (4) using Every's parameters s_1, s_2 and s_3 . In the case of quadratic materials we get

$$c_J = s_1(2s_2 - s_3), \quad c_L = s_1(1 - s_2 + s_3), \quad s_M = 2s_1(1 - s_2), \quad (6)$$

whereas in the case of cubic materials

$$c_J = \frac{s_1}{3}(10s_2 - 6s_3 - 1), \quad c_L = 2\frac{s_1}{3}(1 - s_2), \quad s_M = 2\frac{s_1}{3}(3s_3 - 2s_2 + 2). \quad (7)$$

For both cubic and quadratic materials the first of the inequalities (2) define stability regions in the form of semi-infinite prisms ($s_1 > 0$) with two distinct triangles (STs) at the base in s_2, s_3 -plane.

$$s_1 > 0, s_2 < 1, \quad (8)$$

$$\begin{aligned} 2D : (1 - s_2 + s_3) > 0, (s_2 - s_3/2) > 0, \\ 3D : (1 + 2s_2) > |4s_2 - 3s_3 - 1|, (10s_2 - 6s_3) > 1. \end{aligned} \quad (9)$$

Both stability triangles are lying in the (s_2, s_3) -plane (Fig. 1). The sides of the stability triangles

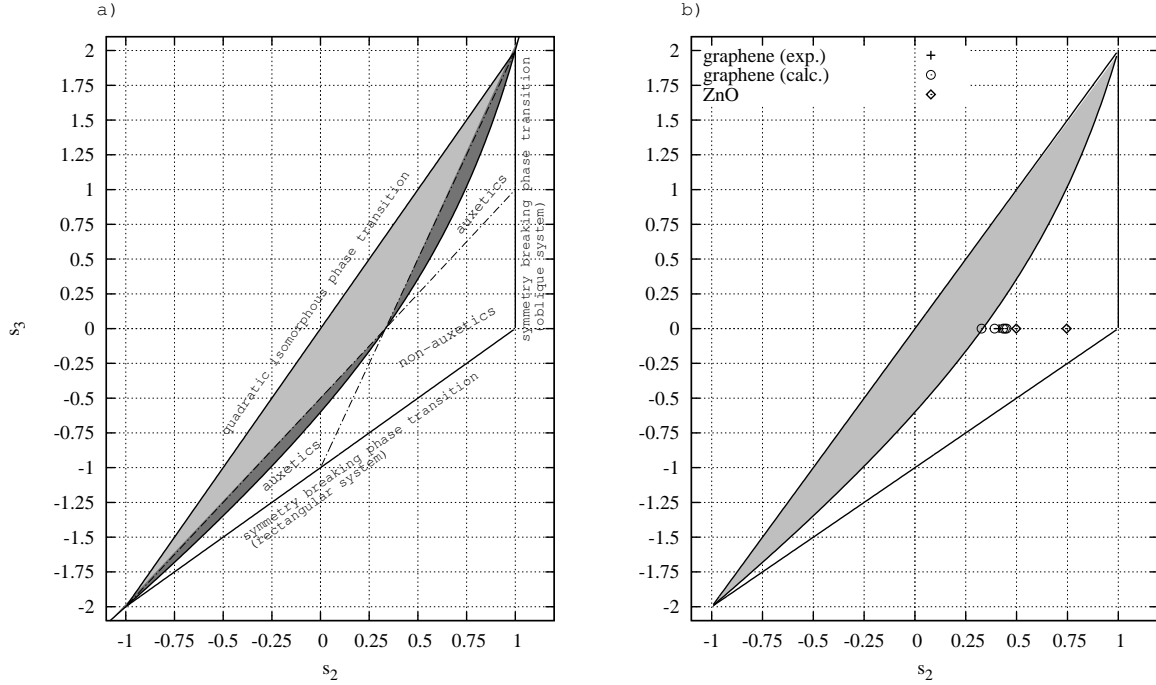


Figure 1. a) Division of the stability triangle for quadratic materials into areas of various auxetic properties. b) The shaded area is the region of complete polycrystalline auxetics. Locations of results for graphene [12], [13] and graphene-like ZnO [14] are indicated.

(STs) are defined by lines

$$\begin{aligned} 2D : s_3^{(2D,1)} &= 2s_2, s_3^{(2D,2)} = s_2 - 1, s_2^{(2D,3)} = 1, \\ 3D : s_3^{(3D,1)} &= 5s_2/3 - 1/6, s_3^{(3D,2)} = 2s_2/3 - 2/3, s_2^{(3d,2)} = 1. \end{aligned} \quad (10)$$

A point of the stability triangle together with the value of s_1 represents an existing or potentially existing crystalline material. For acoustic and elastic characteristics the parameter s_1 is a scaling parameter (cf. [7], [10]). In Figs.1 and 2 we show changes of the division of STs in two regions into various auxetic properties. Points of area with lighter shade represent complete monocrystalline auxetics, whereas in the area with darker shade lie complete polycrystalline auxetics.

For symmetry systems other than cubic and isotropic, as well as for the oblique symmetry system, elastic properties are defined in spaces of dimensions higher than 3. In the case of rectangular symmetry system the space of parameters can be effectively reduced to a 3D space (cf. Appendix). Monocrystalline stable *isotropic* materials are located on the interval of the lines defined by equation $s_3 = 0$ belonging to the appropriate triangle.

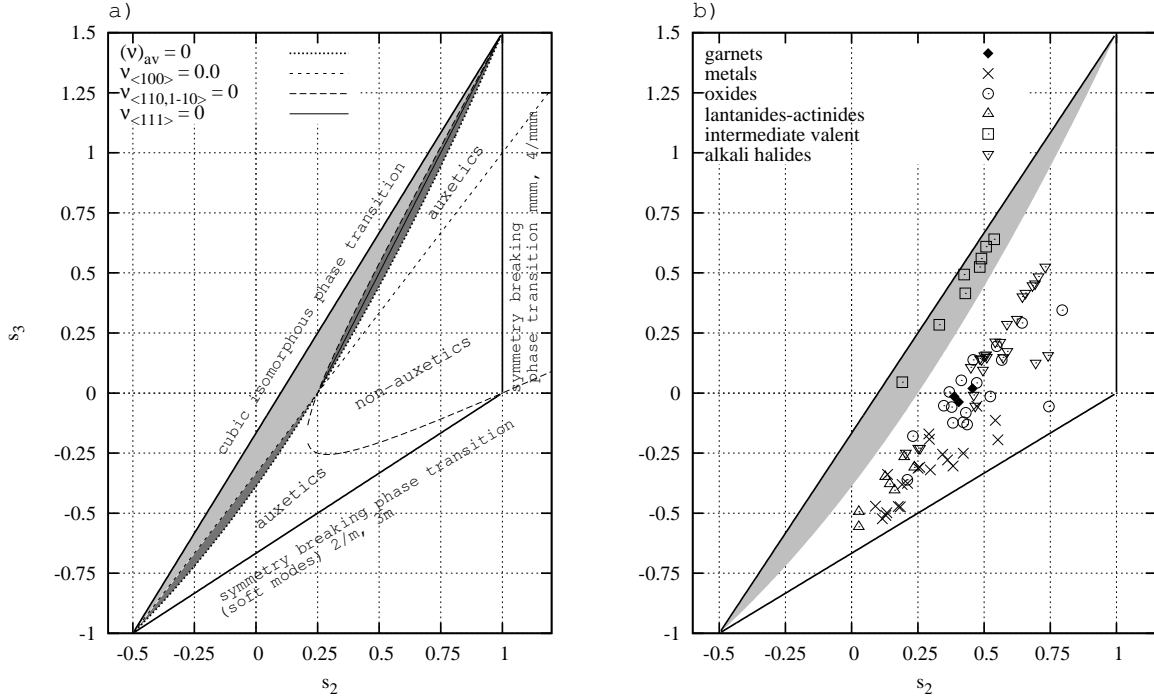


Figure 2. a) Division of the stability triangle for cubic materials into areas of various auxetic properties. b) The shaded area is the region of complete polycrystalline auxetics. Locations of several classes of elastic materials are indicated (cf. [17]).

3. Mechanical characteristics of quadratic and cubic materials

Mechanical properties of an elastic body are characterized by Young's and shear moduli and Poisson's ratio. Recent interest in crystalline materials has made the understanding these characteristics increasingly important. In papers [1] and [2] we derived expressions for them which do not depend on the choice of Cartesian coordinate system. The Young modulus $E(\mathbf{n})$ depends on the (direction) cosines that unit vector \mathbf{n} of the load makes with the crystalline axes. The shear modulus G , as well as the Poisson's ratio ν , additionally depend on the direction cosines of the vector of lateral load \mathbf{m} .

Expressions for these characteristics can be written in terms of the eigenvalues c_J , c_L and c_M . For quadratic materials we obtain

$$E_q(\mathbf{n}) = \frac{2c_J c_L c_M}{c_L c_M + c_J c_M (n_1^2 - n_2^2)^2 + 4c_J c_L n_1^2 n_2^2}, \quad (11)$$

$$G_q(\mathbf{n}, \mathbf{m}) = \frac{1}{2} \frac{c_L c_M}{c_M (m_1 n_1 - m_2 n_2)^2 + c_L (m_1 n_2 + m_2 n_1)^2}, \quad (12)$$

$$-\nu_q(\mathbf{n}, \mathbf{m}) = \frac{c_L c_M + c_J c_M (m_1^2 - m_2^2) (n_1^2 - n_2^2) + 4c_J c_L m_1 m_2 n_1 n_2}{c_L c_M + c_J c_M (n_1^2 - n_2^2)^2 + 4c_J c_L n_1^2 n_2^2}, \quad (13)$$

For cubic materials we get

$$E_c(\mathbf{n}) = \frac{3c_J c_L c_M}{(c_L c_M - c_J c_L + 3c_J c_M) + 3c_J (c_L - c_M) \sum_{i=1}^3 n_i^4}, \quad (14)$$

$$G_c(\mathbf{n}, \mathbf{m}) = \frac{c_J c_L c_M}{c_J c_M + 2c_J (c_L - c_M) \sum_{i=1}^3 m_i^2 n_i^2}, \quad (15)$$

$$- \nu_c(\mathbf{n}, \mathbf{m}) = \frac{c_L (c_M - c_J) + 3c_J (c_L - c_M) \sum_{i=1}^3 m_i^2 n_i^2}{(c_L c_M - c_J c_L + 3c_J c_M) + 3c_J (c_L - c_M) \sum_{i=1}^3 n_i^4}. \quad (16)$$

Note that expressions (11-16) allow one to calculate E , G and ν for a given pair of direction vectors (\mathbf{m}, \mathbf{n}) and for chosen values of s_1 , s_2 and s_3 . In the case of polycrystalline materials numerical calculation provides one with analogous results. Performing calculations for a mesh of points of STs we obtained the appropriate maps [15]. These maps were calculated for $s_1 = 1$.

The direction vector of applied tension \mathbf{n} and direction vector \mathbf{m} in which the lateral expansion/contraction is measured are mutually perpendicular, i.e. $\mathbf{nm} = 0$. For quadratic materials

$$\begin{aligned} n_1 &= m_2 = \cos \varphi, \\ n_2 &= -m_1 = \sin \varphi, \end{aligned} \quad (17)$$

where $0 < \varphi \leq 2\pi$.

In the case of cubic materials [11]

$$\begin{aligned} n_1 &= \cos \alpha \cos \varphi \cos \theta - \sin \alpha \sin \theta, \\ n_2 &= \cos \alpha \cos \varphi \sin \theta + \sin \alpha \cos \theta, \\ n_3 &= -\cos \alpha \sin \varphi, \end{aligned} \quad (18)$$

and

$$\begin{aligned} m_1 &= \sin \varphi \cos \theta, \\ m_2 &= \sin \varphi \sin \theta, \\ m_3 &= \cos \varphi, \end{aligned} \quad (19)$$

where

$$-\pi < \alpha \leq \pi, \quad 0 < \varphi \leq \pi, \quad 0 < \theta \leq 2\pi. \quad (20)$$

4. Mechanical characteristics on the sides of stability triangles

For directions of high symmetry the mechanical characteristics can vanish, signaling phase transitions (cf. [7]). New phases are indicated in Fig. 1.

Consider quadratic materials. For $\mathbf{n}_1^{(q)} = \langle 11 \rangle$, $\mathbf{m}_1^{(q)} = \langle 1\bar{1} \rangle$

$$E_q = \frac{2c_J c_M}{c_J + c_M}, \quad G_q = \frac{c_L}{2}, \quad \nu_q = \frac{c_J - c_M}{c_J + c_M}. \quad (21)$$

This means that for $E_q(\mathbf{n}_1, \mathbf{m}_1)$ vanishes on the top and on the vertical side of ST, whereas $G_q(\mathbf{n}_1, \mathbf{m}_1)$ vanishes on the bottom side of it.

For $\mathbf{n}_2 = \langle 10 \rangle$, $\mathbf{m}_2 = \langle 01 \rangle$

$$E_q = \frac{2c_J c_L}{c_J + c_L}, \quad G_q = \frac{c_M}{2}, \quad \nu_q = \frac{c_J - c_L}{c_J + c_L}. \quad (22)$$

For \mathbf{n}_2 and \mathbf{m}_2 E_q vanishes on the top and bottom side of ST, whereas G_q vanishes on the vertical side.

For $\mathbf{n}_3^{(q)} = \langle n_3^{(q,1)} n_3^{(q,2)} \rangle$ and $\mathbf{m}_3^{(q)} = \langle \bar{n}_3^{(q,2)} n_3^{(q,1)} \rangle$

$$E_q = \frac{4c_J c_L c_M}{2c_L c_M + c_J c_L + c_J c_M}, G_q = \frac{c_L c_M}{c_L + c_M}, \nu_q = \frac{c_J (c_L + c_M) - 2c_L c_M}{c_J (c_L + c_M) + 2c_L c_M}, \quad (23)$$

where $n_3^{(q,1)} = \cos(\pi/8)$ and $n_3^{(q,2)} = \sin(\pi/8)$. This means that $E_q(\mathbf{n}_3^{(q)})$ vanishes on all sides of ST, whereas $G_q(\mathbf{n}_3^{(q)}, \mathbf{m}_3^{(q)})$ vanishes on the bottom and vertical side of ST.

Similar results are valid for cubic materials. For $\mathbf{n}_1^{(c)} = \langle 0 0 1 \rangle$, $\mathbf{m}_1^{(c)} = \langle 1 1 0 \rangle$ Eqs. (14), (15) and (16) give

$$\mathbf{n}_1^{(c)}, \mathbf{m}_1^{(c)} : E_c = \frac{3c_J c_M}{2c_L + c_M}, G_c = \frac{c_L}{2}, \nu_c = \frac{c_J - c_M}{2c_J + c_M}, \quad (24)$$

hence $E_c(\mathbf{n}_1^{(c)}) = 0$ on the top and bottom side of ST, $G_c(\mathbf{n}_1^{(c)}, \mathbf{m}_1^{(c)}) = 0$ on the vertical side of it. For $\mathbf{n}_2^{(c)} = \langle 1 1 0 \rangle$, $\mathbf{m}_2^{(c)} = \langle \bar{1} 1 0 \rangle$ we obtain

$$\begin{aligned} \mathbf{n}_2^{(c)}, \mathbf{m}_2^{(c)} : E_c &= \frac{3c_J c_L c_M}{c_J c_L/2 + 3c_J c_M/2 + c_L c_M/2}, \\ G_c &= \frac{c_M}{2}, -\nu_c = \frac{c_J c_L/2 - 3c_J c_M/2 + c_L c_M}{c_J c_L/2 + 3c_J c_M/2 + c_L c_M}. \end{aligned} \quad (25)$$

For $\mathbf{n}_2^{(c)}$ and $\mathbf{m}_2^{(c)}$ Young's modulus vanishes on all sides of ST, whereas the shear modulus vanishes on the bottom side of it. Finally, for $\mathbf{n}_3^{(c)} = \langle 1 1 1 \rangle$, $\mathbf{m}_3^{(c)} = \langle 0 1 \bar{1} \rangle$

$$\mathbf{n}_3^{(c)}, \mathbf{m}_3^{(c)} : E_c = \frac{3c_J c_L}{2c_J + c_L}, G_c = \frac{3c_L c_M}{2c_L + c_M}, \nu_c = \frac{c_J - c_L}{c_L - 2c_J}. \quad (26)$$

For $\mathbf{n}_3^{(c)}$ and $\mathbf{m}_3^{(c)}$ Young's modulus vanishes on the top and vertical side of ST, the shear modulus vanishes on the vertical and bottom side.

For all considered high symmetry directions Young's and shear moduli are non-negative.

5. Lines of vanishing Poisson's ratio

For a chosen direction \mathbf{n} of load and lateral strain \mathbf{m} the general expressions presented in Sect. 3 allow us to find the lines of vanishing ν that divide the stability triangles into regions of various auxeticity properties. These lines are particularly interesting for \mathbf{n} and \mathbf{m} directed along high symmetry directions.

Consider the quadratic materials. For the following pairs (\mathbf{n}, \mathbf{m}) the condition $\nu_q(\mathbf{m}, \mathbf{n}) = 0$ leads to equations

$$\begin{aligned} (\mathbf{n}_1^{(q)}, \mathbf{m}_1^{(q)}) : s_3(s_2) &= 2(s_2 - 1), \\ (\mathbf{n}_2^{(q)}, \mathbf{m}_2^{(q)}) : s_3(s_2) &= 3s_2/2 - 1/2. \end{aligned} \quad (27)$$

For cubic materials we get

$$\begin{aligned} (\mathbf{n}_1^{(c)}, \mathbf{m}_1^{(c)}) : s_3(s_2) &= 4s_2/3 - 1, \\ (\mathbf{n}_2^{(c)}, \mathbf{m}_2^{(c)}) : s_3(s_2) &= \frac{7}{6}s_2 - \frac{5}{12} \pm \frac{1}{12}\sqrt{68s_2^2 + 20s_2 - 7}, \\ (\mathbf{n}_3^{(c)}, \mathbf{m}_3^{(c)}) : s_3(s_2) &= 2s_2 - 1. \end{aligned} \quad (28)$$

All the above lines of vanishing ν are shown in Fig. 1.

In our papers [3], [4] we introduced the division of the stability triangle into regions of complete auxeticity, auxeticity and non-auxeticity. The above regions are indicated on diagrams in Fig. 1. Inspecting them one can distinguish lines of vanishing ν studied in this section.

Mechanical characteristics of 2- and 3-d cubic polycrystalline materials

Following the assumptions made at the end of Sect. 1 to find the mechanical characteristics of polycrystalline materials one should calculate mean values of expressions defining them. Consider quadratic materials and a function F of the angle φ , then in agreement with definition (17)

$$\langle F \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\varphi F(\varphi). \quad (29)$$

Calculating $\langle E_q \rangle$, $\langle G_q \rangle$ and $\langle \nu_q \rangle$ we obtained

$$\langle E_q \rangle = \frac{4c_J c_L c_M}{\sqrt{[2c_L c_M + c_J (c_L + c_M)]^2 - c_J^2 (c_L - c_M)^2}}, \quad (30)$$

$$\langle G_q \rangle = \sqrt{c_L c_M}/2, \quad (31)$$

$$\langle \nu_q \rangle = 1 - \frac{4c_L c_M}{\sqrt{[2c_L c_M + c_J (c_L + c_M)]^2 - c_J^2 (c_L - c_M)^2}}. \quad (32)$$

Table 1 summarizes the properties of mean values of the mechanical characteristics and eigenvalues c_I ($I = J, L, M$) on sides of ST. These properties align with calculated maps of $\langle E_q \rangle$, $\langle G_q \rangle$ and $\langle \nu_q \rangle$ [15].

Table 1. Values of $\langle E_q \rangle$, $\langle G_q \rangle$ and $\langle \nu_q \rangle$ on the sides of ST. J – top side, M – bottom side, L – vertical side; $U = J, L, M$.

Side	c_U	$\langle E_q \rangle$	$\langle G_q \rangle$	$\langle \nu_q \rangle$
J	0	0	$\sqrt{c_M c_L}/2$	-1
L	0	0	0	1
M	0	0	0	1

In the case of quadratic polycrystalline materials the condition $\langle \nu_q \rangle = 0$ leads to equations of line

$$s_3(s_2) = \frac{3s_2^2 - 10s_2 + 3}{3s_2 - 5}, \quad (33)$$

demarcating the stability triangle to the regions of *complete* auxetics and non-auxetics. In case of cubic materials such a line is found numerically. Inspecting Fig. 2 we note that for polycrystalline 2D and 3D cubic materials the area of region of complete auxeticity is larger than for monocrystalline materials.

In the case of cubic materials and a function F of angles α , φ and θ (cf. Eqs. (18) and (19)) the mean value $\langle F \rangle$ of $F(\alpha, \varphi, \theta)$ is defined as

$$\langle F \rangle = \frac{1}{8\pi^2} \int_{-\pi}^{+\pi} d\alpha \int_0^\pi d\varphi \sin \varphi \int_0^{2\pi} d\theta F(\alpha, \varphi, \theta). \quad (34)$$

Since we consider the model of randomly oriented crystallites, the averaged mechanical characteristics are isotropic. This means, that if $\langle \nu \rangle > 0$, one deals with isotropic non-auxetics, whereas if $\langle \nu \rangle < 0$, a polycrystal is a complete isotropic auxetic. We conclude that in the case of considered models of polycrystals the division of the stability triangles simplifies.

6. Concluding remarks

We have shown that mechanical characteristics of elastic materials expressed in terms of eigenvalues of the stiffness tensor are well suited for the study of their general properties. The simplest model of polycrystalline 2D and 3D cubic materials indicates that some monocrystalline auxetics become complete auxetics in the polycrystalline phase.

Appendix

Elastic properties of rectangular materials are characterized by four stiffnesses C_{11} , C_{22} , C_{12} , C_{66} (cf. [2] and [16]). Initially unstrained rectangular materials are stable if

$$C_{11} > 0, C_{22} > 0, C_{66} > 0, C_{11}C_{22} > C_{12}^2. \quad (35)$$

Introduce four new parameters

$$s_1 = (C_{11} + C_{22})/2 + C_{66}, \quad (36)$$

$$s_2 = [(C_{11} + C_{22})/2 - C_{66}]/s_1, \quad (37)$$

$$s_3 = [(C_{11} + C_{22})/2 - C_{12} - 2C_{66}]/s_1, \quad (38)$$

$$s_4 = (C_{11} - C_{12})/2s_1. \quad (39)$$

Because of inequalities (36)-(39)

$$s_1 > 0, \quad -1 < s_2 < 1, \quad (40)$$

s_4 can be positive and negative.

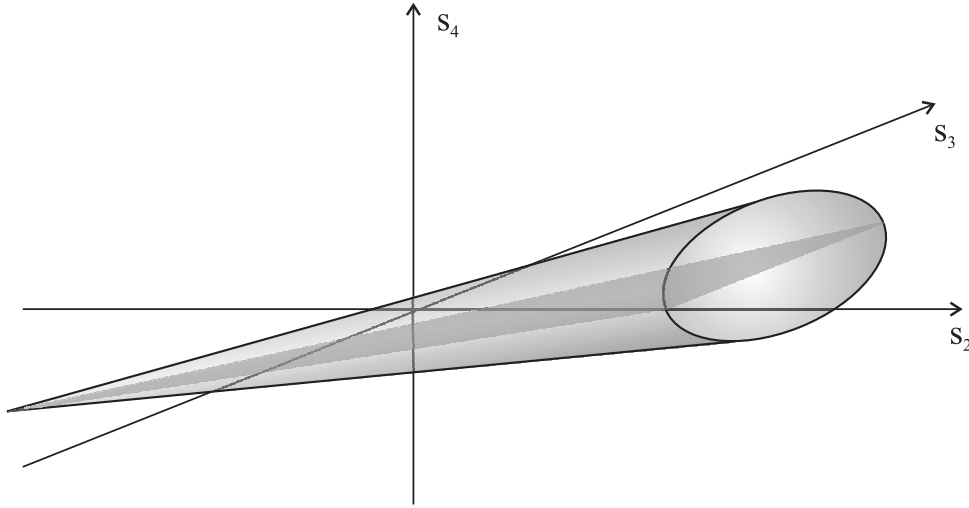


Figure 3. Rectangular materials: mechanical stability region in (s_2, s_3, s_4) -space.

Consider 3D space of parameters s_2 , s_3 , s_4 . In planes $s_2 = \alpha$ ($-1 < \alpha < 1$) the last of inequalities (35) takes the form

$$s_4^2 + (s_3 - d_1)^2 < d_2^2, \quad (41)$$

where $d_1(\alpha) = (3\alpha - 1)/2$, $d_2(\alpha) = (1 + \alpha)/2$. Inequality (41) defines a section of the oblique cone with the apex located at the point $(s_2 = -1, s_3 = -2, s_4 = 0)$. For $-1 < \alpha < 1$ the cross-sections of the cone perpendicular to s_2 axis are circles with radii equal to $d_2(\alpha)$ and centers $(s_2 = \alpha, s_3 = d_1(\alpha), s_4 = 0)$ (Fig. 3). For $s_4 = 0$ the cone (41) reduces to ST defined by Eq. (9).

Conclusions

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